AD-A090 951 GEORGIA INST OF TECH ATLANTA SCHOOL OF PHYSICS F/G 7/4
THE DRIFT, DIFFUSION, AND REACTIONS OF SLOW IONS IN GASES.(U)
FEB 80 E W MCDANIEL, I R GATLAND N00014-76-C-0015
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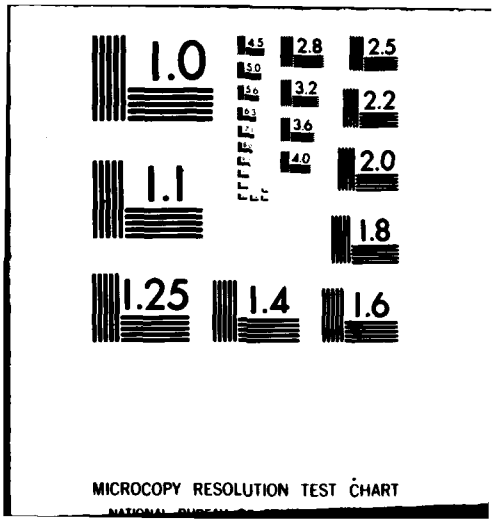
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The Drift, Diffusion, and Reactions of Slow Ions in Gases

O. N. R. FINAL REPORT

Contract N00014-76-C-0015

28 Feb 80

July 1, 1975 - February 28, 1980

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Final rept. 1 Jul 75-28 Feb 80

1. Scientific Problem

The experimental program consisted of measurements of the mobilities and longitudinal diffusion coefficients of ions in various gases at room temperature. By varying the energy parameter (E/N) of the ions, we may vary the average ionic energy from the thermal value at 300°K to about 10 eV. Our measured mobilities and diffusion coefficients are useful in calculations of properties of weakly ionized plasmas. In addition, the mobilities as a function of E/N can be inverted to obtain the interaction potential for the ion-neutral combination involved, and the mobilities are also useful in calculations of the rate of positive ion-negative ion recombination. Rate coefficients measured for ion-molecule reactions play a role in explaining plasma chemistry; ionic transport data are required for the accurate determination of these rate coefficients. Observations on ionic identity and abundances as functions of gas pressure and temperature are particularly important in atmospheric research.

The relevance of ionic transport phenomena to atmospheric problems arises partly from the concomitant transport of charge, mass, momentum, and energy through space. Further, the drift of ions in an electric field can significantly increase the kinetic energy of the ions, and can change their internal excitation energy by ion-molecule collisions. The changes in translational and internal energy can markedly affect the rates of ion-molecule reactions, and subsequently the rates of other kinds of collisions, notably ion-ion and electron-ion recombination, in the atmosphere.

The theoretical program consisted of the calculation of mobilities and diffusion coefficients from given potentials for several particularly interesting ion-neutral systems, the determination of interaction potentials from mobility data using the standard two-temperature theory, investigation of the three-temperature theory in relation to diffusion, and initial studies of polyatomic cases.

From our standpoint the most important use of the mobility data is to generate ion-neutral interaction potentials covering a very wide range of ion-neutral separation distance by inverting the experimental data. The interaction potential for a two-particle system is one of the most fundamental properties of the system. It determines the mutual scattering behavior of the particles and hence the transport properties. The interaction potential also determines many properties of the system that is formed if the two particles can temporarily or permanently combine. In the case of radiative processes, for example, the interaction potentials for the upper and ground states of a neutral diatomic molecule or ion are required for the determination of the wave functions, transition probabilities and spectral features. The standard beam scattering technique used to obtain information about the interaction potential for an ion-neutral system covers a much smaller range of separation distance than does the new method described here. The interaction potentials obtained for the halogen ion-rare gas combinations may have applications in excimer lasers.

We also calculate from our measured drift velocities the zero-field mobilities of these ions in various gases at temperatures ranging from 300°K to $\sim 10^4$ °K by the techniques we have described in Ref. 2 of Section 3.

2. Scientific and Technical Approach

The experiments are performed with a drift tube mass spectrometer, by techniques which permit accurate measurements to be made on individual ionic species even though several species may be simultaneously present and coupled by ion-molecule reactions. The drift tube gas is maintained at room temperature, but the average energy of a given species of ion can be varied from very close to thermal energy up to a maximum of about 10 eV in favorable cases. The average energy of the ions of a given type is determined by the parameter E/N, where E is the intensity of the electrostatic drift field and N is the number density of the neutral gas molecules contained in the drift tube. The measurements are made as a function of E/N.

The basic measurement made is of the arrival time spectra for each separate ionic species in the drift tube. The measurements are made as functions of drift distance, electric field strength (E) in the drift region, number density of gas molecules in the drift tube (N), and the energy parameter (E/N).

The theoretical calculations are concerned with the relation between the ion-neutral interaction potential and the measured values of the mobilities and diffusion coefficients. The calculation of the transport coefficients is based on a moment solution of the appropriate Boltzmann equation with basis functions which reflect the sometimes high random energy derived from the electric field and the non-symmetric character of the ionic velocity. This allows the mobility data to be used to test theoretical potentials and also to serve as an integral part of an iteration technique which determines the interaction potential directly from the data.

3. Results and Publications

The results that we obtained during the period covered by this report are indicated by the titles in the list of publications that follows. Also given in this list are the names of all of the scientific personnel who participated in the research. Of these personnel, the following have obtained their Ph.D. degrees in Physics at the Georgia Institute of Technology: W. F. Morrison (1975), D. R. James (1975), and G. R. Akridge (1976). M. G. Thackston will obtain his Ph.D. degree in December 1980, and D. R. Lamm in 1981.

PUBLICATIONS

1. W. F. Morrison, G. R. Akridge, H. W. Ellis, R. Y. Pai, E. W. McDaniel, L. A. Viehland, and E. A. Mason, "Test of the Li^+ - He Interaction Potential", Jour. Chem. Phys. 63, 2238 (1975).

2. E. A. Mason, L. A. Viehland, H. W. Ellis, D. R. James, and E. W. McDaniel, "The Mobilities of K^+ Ions in Hot Gases", Phys. Fluids 18, 1070 (1975).

3. R. Y. Pai, H. W. Ellis, G. R. Akridge, and E. W. McDaniel, "Longitudinal Diffusion Coefficients of Li^+ and Na^+ Ions in He, Ne, and Ar: Experimental Test of the Generalized Einstein Relation", J. Chem. Phys. 63, 2916 (1975).

4. R. Y. Pai, H. W. Ellis, G. R. Akridge, and E. W. McDaniel, "Generalized Einstein Relation: Application to Ions in Molecular Gases", Phys. Rev. A 12, 1781 (1975).

5. H. W. Ellis, R. Y. Pai, and E. W. McDaniel, "Mobilities of Li^+ and Na^+ Ions in Hydrogen Gas", J. Chem. Phys. 64, 3492 (1976).

6. R. Y. Pai, H. W. Ellis, and E. W. McDaniel, "The Generalized Einstein Relation - Application to Li^+ and Na^+ Ions in Hydrogen Gas", J. Chem. Phys. 64, 4238 (1976).

7. M. G. Thackston, H. W. Ellis, R. Y. Pai, and E. W. McDaniel, "Mobilities of Rb^+ Ions in He, Ne, Ar, H_2, N_2, O_2, and CO_2", J. Chem. Phys. 65, 2037 (1976).

8. H. W. Ellis, M. G. Thackston, R. Y. Pai, and E. W. McDaniel, "Longitudinal Diffusion Coefficients of Rb^+ Ions in He, Ne, Ar, H_2, N_2, O_2, and CO_2", J. Chem. Phys. 65, 3390 (1976).

9. H. W. Ellis, R. Y. Pai, E. W. McDaniel, E. A. Mason, and L. A. Viehland, "Transport Properties of Gaseous Ions Over a Wide Energy Range", Atomic Data and Nuclear Data Tables 17, 177-210 (1976).

10. I. R. Gatland, "Ion-Neutral Interaction Potentials and Gaseous Ion Diffusion Coefficients from Mobility Data", Fourth Int. Conf. on Atomic Physics, Berkeley, Calif., July 1976.

11. E. W. McDaniel, invited paper, "Studies of Ion Plasma Chemistry with Drift Tube Mass Spectrometers", Third International Symposium on Plasma Chemistry, Limoges, France, (July 1977).

12. E. W. McDaniel, invited paper, "Gaseous Ion Transport and Reaction Studies Using Drift Tube Mass Spectrometers", Presented at the U.S.-Japan Joint Seminar on the Glow Discharge and Its Fundamental Processes, Boulder, Colorado, (July 12-15, 1977).

13. I. R. Gatland, W. F. Morrison, H. W. Ellis, M. G. Thackston, E. W. McDaniel, M. H. Alexander, L. A. Viehland, and E. A. Mason, "The Li^+ - He Interaction Potential", Jour. Chem. Phys. 66, 5121 (1977).

14. I. R. Gatland, E. W. McDaniel, H. W. Ellis, M. G. Thackston, F. L. Eisele, and W. M. Pope, "Cs^+ - Kr and Cs^+ - Xe Interaction Potentials", Int. Conf. on the Physics of Electronic and Atomic Collisions, Paris, France, (July 1977).

15. I. R. Gatland, L. A. Viehland, and E. A. Mason, "Tests of Alkali Ion-Inert Gas Interaction Potentials by Gaseous Ion Mobility Experiments", Jour. Chem. Phys. 66, 537 (1977).

16. M. G. Thackston, F. L. Eisele, H. W. Ellis, and E. W. McDaniel, "Mobilities of Cs^+ Ions in Molecular Gases: H_2, N_2, O_2, CO, and CO_2", Jour. Chem. Phys. 67, 1276 (1977).

17. F. L. Eisele, M. G. Thackston, W. M. Pope, I. R. Gatland, H. W. Ellis, and E. W. McDaniel, "Experimental Test of the Generalized Einstein Relation for Cs^+ Ions in Molecular Gases: H_2, N_2, O_2, CO, and CO_2", Jour. Chem. Phys. 67, 1278 (1977).

18. M. G. Thackston, F. L. Eisele, W. M. Pope, H. W. Ellis, and E. W. McDaniel, "Further Tests of the Generalized Einstein Relation: Cs^+ Ions in Ar, Kr, and Xe", Jour. Chem. Phys. 68, 3950 (1978).

19. W. M. Pope, H. W. Ellis, F. L. Eisele, M. G. Thackston, E. W. McDaniel, and R. A. Langley, "Mobilities and Longitudinal Diffusion Coefficients for Cs^+ Ions in He and Ne Gas", Jour. Chem. Phys. 68, 4761 (1978).

20. H. W. Ellis, E. W. McDaniel, D. L. Albritton, L. A. Viehland, S. L. Lin, and E. A. Mason, "Transport Properties of Gaseous Ions Over a Wide Energy Range - Part II", Atomic Data and Nuclear Data Tables 22, 179-217 (1978).

21. I. R. Gatland, M. G. Thackston, W. M. Pope, F. L. Eisele, H. W. Ellis, and E. W. McDaniel, "Mobilities and Interaction Potentials for Cs^+ - Ar, Cs^+ - Kr, and Cs^+ - Xe", Jour. Chem. Phys. 68, 2775 (1978).

22. I. R. Gatland, D. R. Lamm, M. G. Thackston, W. M. Pope, F. L. Eisele, H. W. Ellis, and E. W. McDaniel, "Mobilities and Interaction Potentials for Rb^+ - Ar, Rb^+ - Kr, and Rb^+ - Xe", Jour. Chem. Phys. 69, 4951 (1978).

23. W. M. Pope, F. L. Eisele, M. G. Thackston, and E. W. McDaniel, "Longitudinal Diffusion Coefficients and Test of the Generalized Einstein Relation for Rb^+ - Kr, Rb^+ - Xe, K^+ - Kr, and K^+ - Xe", Jour. Chem. Phys. 69, 3874 (1978).

24. M. G. Thackston, F. L. Eisele, W. M. Pope, H. W. Ellis, I. R. Gatland, and E. W. McDaniel, "Mobility of Cl^- Ions in Ne, Ar, and Kr", J. Chem. Phys. 70, 3996 (1979).

25. F. L. Eisele, M. G. Thackston, W. M. Pope, H. W. Ellis, and E. W. McDaniel, "Longitudinal Diffusion Coefficients and the Generalized Einstein Relation for Cl^- Ions in Ne, Ar, Kr, and Xe", Jour. Chem. Phys. 70, 5918 (1979).

26. S. L. Lin, I. R. Gatland, and E. A. Mason, "Mobility and Diffusion of Protons and Deuterons in Helium - a Runaway Effect", J. Phys. B 12, 4179 (1979).

27. M. G. Thackston, F. L. Eisele, W. M. Pope, H. W. Ellis, and E. W. McDaniel, "Mobilities and Longitudinal Diffusion Coefficients for F^- Ions in Kr and Xe", Jour. Chem. Phys. 73, 1477 (1980).

28. M. G. Thackston, M. S. Sanchez, G. W. Neeley, W. M. Pope, F. L. Eisele, I. R. Gatland, and E. W. McDaniel, "Mobilities and Longitudinal Diffusion Coefficients for Na^+ Ions in Kr and Xe", Jour. Chem. Phys. 73, 2012 (1980).

29. M. G. Thackston, F. L. Eisele, W. M. Pope, H. W. Ellis, E. W. McDaniel, and I. R. Gatland, "Mobility of Cl^- Ions in Xe Gas and the Cl^- - Xe Interaction Potential", Jour. Chem. Phys. 73, 3183 (1980).

30. E. W. McDaniel, "Ionic Transport Phenomena and Their Applications", invited paper presented at Sixth Int. Conf. on Atmospheric Electricity, Manchester, England, July 28 - August 1, 1980. Conf. Proceedings to be published (1981).

31. H. S. W. Massey, B. Bederson, and E. W. McDaniel (Eds.), Applied Atomic Collision Physics, 4 Vols., Academic, New York, in press.

32. D. R. Lamm, M. G. Thackston, F. L. Eisele, H. W. Ellis, J. R. Twist, W. M. Pope, I. R. Gatland, and E. W. McDaniel, "Mobilities and Interaction Potentials for K^+ - Ar, K^+ - Kr, and K^+ - Xe", Jour. Chem. Phys., in press.

33. M. G. Thackston, M. S. Sanchez, G. W. Neeley, W. M. Pope, J. R. Twist, and E. W. McDaniel, "The Mobilities and Longitudinal Diffusion Coefficients of Li^+ Ions in Kr and Xe", to be submitted to Jour. Chem. Phys.

34. J. R. Twist, F. L. Eisele, M. G. Thackston, F. B. Holleman, R. Chelf, D. R. Lamm, I. R. Gatland, and E. W. McDaniel, "The Mobilities and Longitudinal Diffusion Coefficients of Br^- Ions in Ne, Ar, Kr, and Xe", to be submitted to Jour. Chem. Phys.

35. H. W. Ellis, E. W. McDaniel, and E. A. Mason, "Transport Properties of Gaseous Ions - Part III", to be submitted to Atomic Data and Nuclear Data Tables.

36. E. W. McDaniel, and E. A. Mason, The Mobility and Diffusion of Ions in Gases (2nd. Ed.), Wiley, New York, in preparation.

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SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER	2. GOVT ACCESSION NO. AD-A090	3. RECIPIENT'S CATALOG NUMBER 951
4. TITLE (and Subtitle) Final Report		5. TYPE OF REPORT & PERIOD COVERED Final July 1, 1975 - Feb. 28, 1980
		6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) E. W. McDaniel and I. R. Gatland		8. CONTRACT OR GRANT NUMBER(s) N00014-76-C-0015
9. PERFORMING ORGANIZATION NAME AND ADDRESS School of Physics Georgia Institute of Technology Atlanta, Ga. 30332		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS NR014-314
11. CONTROLLING OFFICE NAME AND ADDRESS Office of Naval Research Physics Program Office Arlington, Va. 22217		12. REPORT DATE March 30, 1980
		13. NUMBER OF PAGES 6
14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office)		15. SECURITY CLASS. (of this report) Unclassified
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Ionic Mobilities
Diffusion Coefficients
Interaction Potentials
Alkali Ions
Halogen Ions
Noble Gases

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

The Georgia Tech program of research on ionic transport in gases is described. Experimental measurements of ionic mobilities and diffusion coefficients are discussed. The use of the mobility data to obtain ion-neutral interaction potentials is described. References are given for publications covering this report period.

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